Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[di-μ_4-benzene-1,4-dicarboxylato-μ_6-succinato-disamarium(III)]

Qin He* and Bao-Jun Huang

Department of Chemistry, Xuchang University, Xuchang 461000, People's Republic of China
Correspondence e-mail: qhe.xcu@163.com

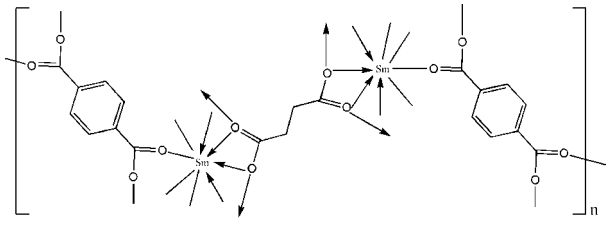
Received 25 October 2007; accepted 31 October 2007

Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.004 Å; R factor = 0.021; wR factor = 0.047; data-to-parameter ratio = 16.3.

The title compound, $[Sm_2(C_4H_4O_4)(C_8H_4O_4)_2]_n$, has been hydrothermally synthesized. The Sm atom is coordinated by four O atoms from four benzene-1,4-dicarboxylate (BDC) ligands and four O atoms from three succinate anions in a distorted square antiprismatic geometry. The antiprisms are bridged by the BDC and succinate ligands, forming a three-dimensional network. The succinate ion is located on a centre of inversion.

Related literature

For related literature, see: Li & Wang (2005); Li *et al.* (2006); He *et al.* 2006); Wang & Li (2005).



Experimental

Crystal data

$[Sm_2(C_4H_4O_4)(C_8H_4O_4)_2]$
M_r = 745.00
Orthorhombic, *Pbca*
a = 13.9896 (2) Å
b = 6.8923 (1) Å
c = 21.8748 (3) Å
V = 2109.18 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 5.58 mm^{-1}
T = 291 (2) K
0.30 × 0.24 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.215, T_{max} = 0.455
11742 measured reflections
2521 independent reflections
2028 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.047
S = 1.03
2521 reflections
155 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.66 e Å^{-3}
$\Delta\rho_{min}$ = −0.65 e Å^{-3}

Table 1
Selected bond lengths (Å).

Sm—O1	2.351 (2)	Sm—O5^{iv}	2.501 (2)
Sm—O2^{i}	2.298 (2)	Sm—O5	2.591 (2)
Sm—O3^{ii}	2.359 (2)	Sm—O6^{v}	2.450 (2)
Sm—O4^{iii}	2.377 (2)	Sm—O6	2.542 (2)

Symmetry codes: (i) $-x+2, -y+2, -z+1$; (ii) $-x+\frac{3}{2}, -y+2, z-\frac{1}{2}$; (iii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (iv) $-x+\frac{3}{2}, y-\frac{1}{2}, z$; (v) $-x+\frac{3}{2}, y+\frac{1}{2}, z$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2044).

References

Bruker (1998). *SMART* (Version 5.16), *SAINT* (Version 6.01) and *SHELXTL* (Version 6.14). Bruker AXS Inc., Madison, Wisconsin, USA.
He, Q., Zi, J.-F. & Zhang, F.-J. (2006). *Acta Cryst.* E**62**, m997–m998.
Li, Z.-F. & Wang, C.-X. (2005). *Acta Cryst.* E**61**, m2689–m2690.
Li, Z.-F., Wang, C.-X., Li, Y., Cai, D.-J. & Xiao, Y.-J. (2006). *Acta Cryst.* E**62**, m251–m252.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Wang, C.-X. & Li, Z.-F. (2005). *Acta Cryst.* E**61**, m2212–m2213.

 doi:10.1107/S1600536807055006

supplementary materials

Acta Cryst. (2007). E**63**, m2923 [**doi:10.1107/S1600536807055006**]

Poly[di-μ_4-benzene-1,4-dicarboxylato-μ_6-succinato-disamarium(III)]

Q. He and B.-J. Huang

Comment

The title compound, (I), is isostructural with its $[M_2(C_8H_4O_4)_2(C_4H_4O_4)]_n$ [*M* = Gd (Wang & Li, 2005), Dy ((Li & Wang, 2005), Nd (Li *et al.*, 2006), Er (He *et al.*, 2006)] analogues. As depicted in Fig.1, The Sm^{3+} ion is located at the center of a distorted square antiprism geometry and is coordinated by four O atoms from four BDC and four O atoms from three succinate anions. The Sm—O bond distances range from 2.298 (2) to 2.591 (2) Å.

In (I), the succinate ligand is located on an inversion centre and functions as an octadentate ligand, bis-chelating two Sm atoms with each O atom bridging to another Sm atom. In this mode, the Sm atoms are linked into a two-dimensional polymeric sheet parallel to the (001) plane. These sheets are in turn bridged *via* BDC ligands, forming a three-dimensional framework.

Experimental

A mixture of $SmCl_3·6H_2O$ (2.00 mmol, 0.73 g), benzene-1,4-dicarboxylic acid (1.0 mmol, 0.16 g), succinic acid (1.0 mmol, 0.10 g), NaOH (6.0 ml, 1 mol/*L*) and H_2O (20.0 ml) was heated in a 35 ml stainless steel reactor with a Teflon liner at 453 K for 48 h. The column-like crystals were filtered and washed with ethanol. Yield: 5% based on Sm.

Refinement

H atoms were included at calculated positions and treated as riding atoms, with C—H distances of 0.93–0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$].

Figures

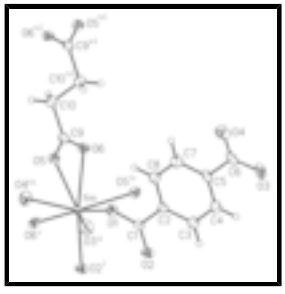


Fig. 1. The coordination environment of the Sm atom, with the atom-numbering scheme, showing displacement ellipsoids drawn at the 50% probability level. Symmetry codes: (i) 2 − *x*, 2 − *y*, 1 − *z*; (ii) 3/2 − *x*, 2 − *y*, *z* − 1/2; (iii) *x*, 3/2 − *y*, *z* − 1/2; (iv) 3/2 − *x*, *y* − 1/2, *z*; (v) 3/2 − *x*, *y* + 1/2, *z*; (vi) 1 − *x*, 2 − *y*, 1 − *z*.

Poly[di-μ4-benzene-1,4-dicarboxylato-μ6-succinato-disamarium(III)]

Crystal data

$[Sm_2(C_4H_4O_4)(C_8H_4O_4)_2]$	F_{000} = 1408
M_r = 745.00	D_x = 2.346 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 258 reflections
a = 13.9896 (2) Å	θ = 3.3–26.7º
b = 6.8923 (1) Å	μ = 5.58 mm^{-1}
c = 21.8748 (3) Å	*T* = 291 (2) K
V = 2109.18 (5) Å^3	Column, colorless
Z = 4	0.30 × 0.24 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer	2521 independent reflections
Radiation source: fine-focus sealed tube	2028 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.034
T = 291(2) K	θ_{max} = 28.0º
φ and ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −16→18
T_{min} = 0.215, T_{max} = 0.455	*k* = −8→9
11742 measured reflections	*l* = −25→28

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.021	$w = 1/[\sigma^2(F_o^2) + (0.010P)^2 + 2.1343P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.047	$(\Delta/\sigma)_{max}$ = 0.010
S = 1.03	$\Delta\rho_{max}$ = 0.66 e Å^{-3}
2521 reflections	$\Delta\rho_{min}$ = −0.65 e Å^{-3}
155 parameters	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.00015 (4)
Secondary atom site location: difference Fourier map	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sm	0.831769 (9)	1.01978 (2)	0.445280 (7)	0.01351 (6)
O1	0.86274 (16)	1.0413 (3)	0.55071 (9)	0.0213 (5)
O2	1.00773 (15)	0.9231 (3)	0.56802 (10)	0.0226 (5)
C1	0.9245 (2)	0.9670 (4)	0.58552 (13)	0.0162 (6)
C2	0.8979 (2)	0.9258 (5)	0.65030 (13)	0.0179 (6)
C3	0.8072 (2)	0.9726 (5)	0.67140 (16)	0.0275 (8)
H3A	0.7629	1.0297	0.6452	0.033*
C4	0.7827 (2)	0.9339 (5)	0.73188 (15)	0.0283 (8)
H4A	0.7220	0.9658	0.7460	0.034*
C5	0.8480 (2)	0.8480 (5)	0.77128 (15)	0.0234 (7)
C6	0.8204 (2)	0.7994 (5)	0.83569 (15)	0.0244 (7)
C7	0.9386 (2)	0.8012 (6)	0.74961 (16)	0.0310 (8)
H7A	0.9828	0.7441	0.7757	0.037*
C8	0.9635 (2)	0.8391 (5)	0.68950 (15)	0.0276 (8)
H8A	1.0241	0.8065	0.6754	0.033*
O3	0.74192 (17)	0.8604 (4)	0.85596 (10)	0.0314 (6)
O4	0.87809 (19)	0.6959 (4)	0.86582 (11)	0.0336 (6)
O5	0.67416 (15)	1.1773 (3)	0.48285 (10)	0.0213 (5)
O6	0.66547 (15)	0.8740 (3)	0.45425 (11)	0.0247 (5)
C9	0.6247 (2)	1.0309 (5)	0.46912 (17)	0.0234 (7)
C10	0.5163 (2)	1.0420 (5)	0.46982 (17)	0.0292 (8)
H10A	0.4954	1.1757	0.4661	0.035*
H10B	0.4897	0.9682	0.4361	0.035*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sm	0.01370 (9)	0.01523 (10)	0.01160 (9)	−0.00074 (5)	−0.00012 (5)	−0.00132 (6)
O1	0.0238 (11)	0.0261 (13)	0.0141 (12)	0.0017 (9)	−0.0008 (8)	0.0010 (10)
O2	0.0178 (11)	0.0329 (13)	0.0171 (11)	−0.0004 (10)	0.0051 (9)	0.0015 (10)
C1	0.0209 (15)	0.0168 (16)	0.0109 (15)	−0.0034 (11)	0.0016 (11)	0.0003 (12)
C2	0.0233 (15)	0.0170 (17)	0.0133 (15)	−0.0002 (12)	0.0024 (12)	0.0035 (12)

C3	0.0269 (16)	0.034 (2)	0.0213 (18)	0.0129 (14)	0.0048 (13)	0.0048 (15)
C4	0.0275 (18)	0.037 (2)	0.0208 (17)	0.0083 (15)	0.0108 (14)	0.0023 (16)
C5	0.0367 (19)	0.0186 (17)	0.0151 (16)	0.0012 (13)	0.0066 (14)	0.0037 (13)
C6	0.0316 (18)	0.0246 (18)	0.0170 (16)	−0.0059 (14)	0.0046 (14)	−0.0003 (14)
C7	0.0291 (18)	0.042 (2)	0.0214 (18)	0.0072 (15)	0.0010 (14)	0.0135 (17)
C8	0.0222 (16)	0.040 (2)	0.0202 (18)	0.0047 (14)	0.0049 (13)	0.0100 (16)
O3	0.0328 (14)	0.0406 (16)	0.0208 (12)	−0.0007 (11)	0.0086 (10)	−0.0023 (11)
O4	0.0457 (15)	0.0327 (15)	0.0226 (13)	0.0043 (12)	0.0087 (11)	0.0107 (11)
O5	0.0219 (12)	0.0163 (12)	0.0257 (13)	−0.0014 (9)	0.0024 (9)	−0.0031 (9)
O6	0.0191 (11)	0.0155 (12)	0.0397 (15)	0.0029 (9)	0.0081 (10)	−0.0011 (10)
C9	0.0202 (16)	0.0201 (19)	0.0299 (19)	−0.0007 (13)	0.0100 (13)	0.0004 (15)
C10	0.0306 (19)	0.023 (2)	0.034 (2)	0.0050 (14)	0.0060 (15)	0.0029 (16)

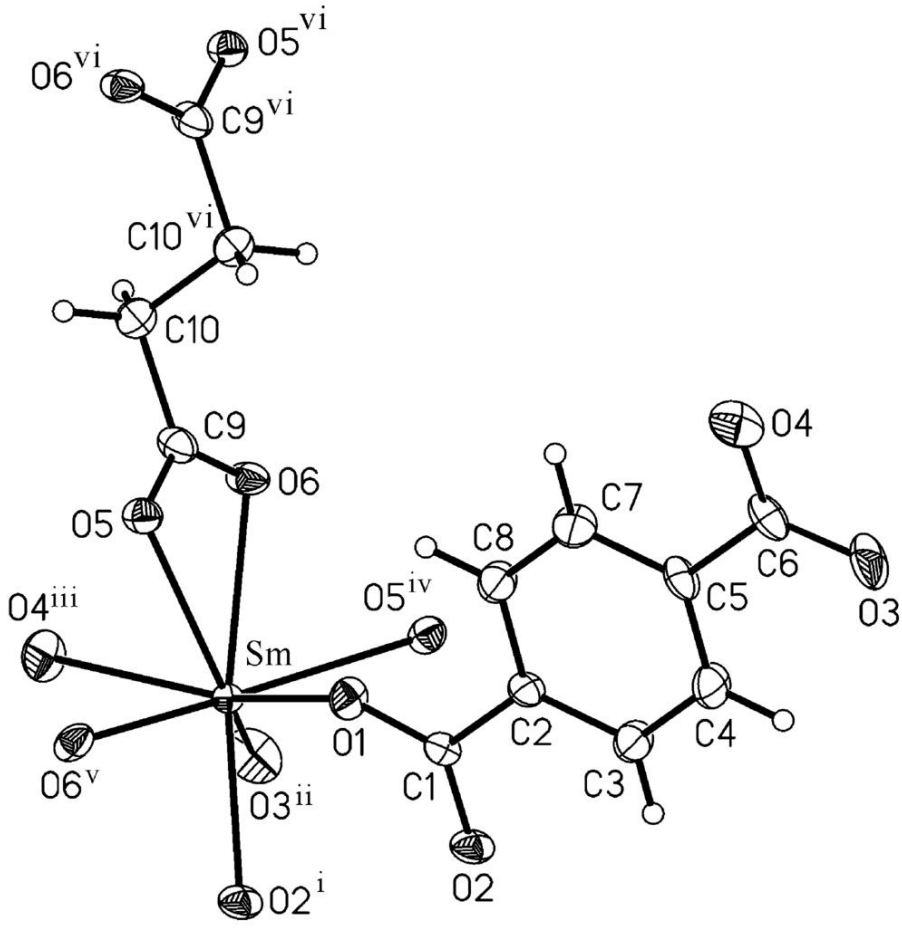
Geometric parameters (Å, °)

Sm—O1	2.351 (2)	C4—C5	1.388 (5)
Sm—O2^{i}	2.298 (2)	C4—H4A	0.9300
Sm—O3^{ii}	2.359 (2)	C5—C7	1.391 (5)
Sm—O4^{iii}	2.377 (2)	C5—C6	1.499 (4)
Sm—O5^{iv}	2.501 (2)	C6—O3	1.257 (4)
Sm—O5	2.591 (2)	C6—O4	1.262 (4)
Sm—O6^{v}	2.450 (2)	C7—C8	1.385 (4)
Sm—O6	2.542 (2)	C7—H7A	0.9300
O1—C1	1.260 (4)	C8—H8A	0.9300
O2—C1	1.263 (4)	O5—C9	1.260 (4)
C1—C2	1.492 (4)	O6—C9	1.265 (4)
C2—C3	1.389 (4)	C9—C10	1.519 (5)
C2—C8	1.391 (4)	C10—C10^{vi}	1.512 (7)
C3—C4	1.392 (5)	C10—H10A	0.9700
C3—H3A	0.9300	C10—H10B	0.9700
O2^{i}—Sm—O1	86.17 (8)	C3—C2—C8	119.9 (3)
O2^{i}—Sm—O3^{ii}	105.20 (8)	C3—C2—C1	119.9 (3)
O1—Sm—O3^{ii}	150.58 (8)	C8—C2—C1	120.2 (3)
O2^{i}—Sm—O4^{iii}	75.42 (8)	C2—C3—C4	119.7 (3)
O1—Sm—O4^{iii}	134.93 (9)	C2—C3—H3A	120.1
O3^{ii}—Sm—O4^{iii}	74.49 (9)	C4—C3—H3A	120.1
O2^{i}—Sm—O6^{v}	79.86 (8)	C5—C4—C3	120.7 (3)
O1—Sm—O6^{v}	81.71 (8)	C5—C4—H4A	119.7
O3^{ii}—Sm—O6^{v}	73.99 (8)	C3—C4—H4A	119.7
O4^{iii}—Sm—O6^{v}	132.66 (8)	C4—C5—C7	119.1 (3)
O2^{i}—Sm—O5^{iv}	103.63 (8)	C4—C5—C6	120.7 (3)
O1—Sm—O5^{iv}	75.12 (7)	C7—C5—C6	120.2 (3)
O3^{ii}—Sm—O5^{iv}	126.04 (8)	O3—C6—O4	124.3 (3)
O4^{iii}—Sm—O5^{iv}	70.06 (8)	O3—C6—C5	118.8 (3)
O6^{v}—Sm—O5^{iv}	156.20 (8)	O4—C6—C5	116.9 (3)

O2^{i}—Sm—O6	166.37 (7)	C8—C7—C5	120.6 (3)
O1—Sm—O6	96.77 (8)	C8—C7—H7A	119.7
O3^{ii}—Sm—O6	78.60 (8)	C5—C7—H7A	119.7
O4^{iii}—Sm—O6	93.37 (8)	C7—C8—C2	120.0 (3)
O6^{v}—Sm—O6	113.71 (6)	C7—C8—H8A	120.0
O5^{iv}—Sm—O6	64.61 (7)	C2—C8—H8A	120.0
O2^{i}—Sm—O5	143.10 (7)	C6—O3—Sm^{vii}	142.3 (2)
O1—Sm—O5	79.60 (7)	C6—O4—Sm^{viii}	124.1 (2)
O3^{ii}—Sm—O5	75.17 (8)	C9—O5—Sm^{v}	131.3 (2)
O4^{iii}—Sm—O5	136.53 (8)	C9—O5—Sm	93.21 (18)
O6^{v}—Sm—O5	64.56 (7)	Sm^{v}—O5—Sm	108.63 (8)
O5^{iv}—Sm—O5	105.25 (6)	C9—O6—Sm^{iv}	151.6 (2)
O6—Sm—O5	50.38 (7)	C9—O6—Sm	95.45 (18)
O2^{i}—Sm—C9	168.31 (9)	Sm^{iv}—O6—Sm	111.92 (8)
O1—Sm—C9	90.34 (9)	O5—C9—O6	119.9 (3)
O3^{ii}—Sm—C9	73.00 (9)	O5—C9—C10	120.4 (3)
O4^{iii}—Sm—C9	114.45 (9)	O6—C9—C10	119.8 (3)
O6^{v}—Sm—C9	88.60 (8)	O5—C9—Sm	61.49 (16)
O5^{iv}—Sm—C9	86.19 (8)	O6—C9—Sm	59.24 (15)
O6—Sm—C9	25.31 (8)	C10—C9—Sm	170.3 (3)
O5—Sm—C9	25.30 (8)	C10^{vi}—C10—C9	106.8 (4)
C1—O1—Sm	133.9 (2)	C10^{vi}—C10—H10A	110.4
C1—O2—Sm^{i}	154.0 (2)	C9—C10—H10A	110.4
O1—C1—O2	123.1 (3)	C10^{vi}—C10—H10B	110.4
O1—C1—C2	118.7 (3)	C9—C10—H10B	110.4
O2—C1—C2	118.2 (3)	H10A—C10—H10B	108.6

Symmetry codes: (i) −*x*+2, −*y*+2, −*z*+1; (ii) −*x*+3/2, −*y*+2, *z*−1/2; (iii) *x*, −*y*+3/2, *z*−1/2; (iv) −*x*+3/2, *y*−1/2, *z*; (v) −*x*+3/2, *y*+1/2, *z*; (vi) −*x*+1, −*y*+2, −*z*+1; (vii) −*x*+3/2, −*y*+2, *z*+1/2; (viii) *x*, −*y*+3/2, *z*+1/2.

Fig. 1


O5vi
O6vi
C9vi
C10vi
C10
C9
O6
O5
O4iii
Sm
O5iv
O6v
O3ii
O2i
O1
C1
O2
C2
C3
C4
C5
C6
C7
C8
O4
O3